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# A second-order theory for piezoelectricity with $6mm$ and $m3$ crystal classes

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## Abstract

The present paper concentrates on the basic equations of three-dimensional problems for nonlinear piezoelectric materials of hexagonal systems with symmetry class  $6mm$  and of cubic systems with symmetry class  $m3$ . Emphasis is placed on developing the nonlinear constitutive relations between extended traction (including elastic stress and polarization) and extended strain (including elastic strain and electric field). The corresponding one-dimensional mathematical models for piezoelectric ceramic with symmetry classes  $6mm$  and  $m3$  are also given. Numerical examples are also carried out for the impact problem to show the important effect of the piezoelectric nonlinearity on the stress wave. Therefore, the derived concise equations can directly be applied to evaluate the nonlinear piezoelectric effects of piezoelectricity by the nonlinear finite element method.

## 1. Introduction

The phenomenon of piezoelectricity was first discovered by the Curie brothers, Pierre and Jacques, in 1880. Piezoelectricity is currently enjoying a great resurgence in both fundamental research and technical applications (Chen 1971, Chizhikov *et al* 1982, Maugin 1988, Ashida and Tauchert 1998, Chandrasekharaiah 1998). Although the behavior of piezoelectric materials in non-structural applications has been investigated extensively, the treatment is often simplistic. In particular, most of the achievements have only been made in the frame of linear constitutive relations.

The rapid development of computer science and nonlinear finite element applications reveals the importance of establishing the nonlinear basic theory for piezoelectricity. Nelson (1978), Toupin (1983), Tiersten (1981) studied the nonlinear theory of dielectrics. Norwood *et al* (1991), Kulkarni and Hanagud (1991) used a Neo-Hookean constitutive relation to model the response of piezoelectric ceramics. Pai *et al* (1992) considered the dependence of the piezoelectric strain parameters upon the strain in formulating a plate theory of piezoelectric laminates. Joshi (1992) considered the nonlinear constitutive relations for piezoelectric materials, where a concise expression was given. Tiersten (1993) investigated

the nonlinear problems of thin plates subjected to large driving voltages. However, most of these studies considered only the case of small deformations, and second-order items were often neglected. Later on, based on the theory of invariants, from invariant polynomial constitutive relations, Yang and Batra (1995) investigated the second-order theory for piezoelectric materials with symmetry class  $6mm$  and class  $mm2$ , where only nine independent stiffness constants were introduced for the nonlinear items.

In this paper, we develop the basic constitutive equations for three-dimensional nonlinear problems of piezoelectric materials. The polynomial constitutive relations for the  $6mm$  crystal class and  $m3$  crystal class are derived using an invariant integrity basis. Furthermore all the basic equations are specialized to those corresponding to the one-dimensional model. This one-dimensional model is then solved by implementing the governing equations in the COMSOL Multiphysics software (COMSOL 2008). These numerical examples of the impact problem show the influence of the piezoelectric nonlinearity on the stress wave. Since the present theory is not restricted to small applied loads or electric fields, it should therefore be very useful to researchers for the investigation of the mechanics and physics of piezoelectricity undergoing large nonlinear deformations (Cheng 1996, Hokstad 2004).

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## 2. Statement of dynamic problems for a nonlinear piezoelectric material

Let the coordinates of a material particle with respect to a rectangular Cartesian coordinate system be  $X_K$  in the reference configuration (undeformed configuration) and its spatial coordinates in the current configuration (deformed configuration) be  $x_k$ .

### 2.1. Governing equations

For a nonlinear piezoelectric material, in the absence of body force and free charge density, the moving equation and the quasistatic approximation to Maxwell's equations in the reference configuration can be written as (Yang and Batra 1995, Pao 1978, Kiral and Eringen 1990)

$$[T_{KL}x_{k,L} + JF_{Kl}^{-1}\varepsilon_0(F_{Mk}^{-1}F_{Nl}^{-1} - \frac{1}{2}F_{Mm}^{-1}F_{Nm}^{-1}\delta_{kl})E_ME_N]_{,K} = \rho_0\delta_{kK}\ddot{u}_K, \quad (1)$$

$$\Pi_{K,K} + J\varepsilon_0F_{Kk}^{-1}(F_{Mk}^{-1}E_M)_{,K} = 0, \quad (2)$$

where

$$J = \det(\mathbf{F}), \quad (3)$$

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}, \quad (4)$$

$T_{KL}$  is the second Piola–Kirchhoff (PK2) stress tensor,  $u_K$  the mechanical displacement vector,  $\Pi_K$  the material electric polarization,  $E_K$  the electric field,  $\rho_0$  the mass density in the reference configuration,  $\varepsilon_0$  the permittivity of free space,  $\delta_{kK}$  the shifter, and  $\delta_{kl}$  the Kronecker delta. Throughout this paper, a repeated index implies summation over the range of the index, and a comma followed by  $K(i)$  implies partial differentiation with respect to  $X_K(x_i)$ . A dot above a quantity signifies its material time derivative. In addition, the PK2 stress tensor  $T_{KL}$  can be written as

$$T_{KL} = JX_{K,k}X_{L,l}(\sigma_{kl} + P_kE_l), \quad (5)$$

where  $\sigma_{kl}$ ,  $P_k$  and  $E_k$  are, respectively, the Cauchy stress, electric polarization, and electric field in the current configuration.

For an isothermal or adiabatic process, in the material configuration, the energy density function in the absence of heat conduction or heat sources can be defined as (Pao 1978)

$$\Sigma = \Sigma(\Gamma_{KL}, E_K), \quad (6)$$

where  $\Gamma_{KL}$  is the Green–Lagrange strain tensor, and  $E_K$  the electric field in the material form.

Also, the displacement–strain and electric potential–electric field can be expressed as

$$\Gamma_{KL} = \frac{1}{2}(x_{k,K}x_{k,L} - \delta_{KL}) = \frac{1}{2}(u_{K,L} + u_{L,K} + u_{M,K}u_{M,L}), \quad (7)$$

$$E_K = -\phi_{,K}. \quad (8)$$

In addition, the basic equations (1) and (2) are accompanied by the following constitutive relations (Pao 1978)

$$T_{KL} = \frac{\partial \Sigma}{\partial \Gamma_{KL}}, \quad (9)$$

$$\Pi_K = -\frac{\partial \Sigma}{\partial E_K}. \quad (10)$$

### 2.2. Boundary and initial conditions

#### (a) Mechanical boundary conditions

$$u_K = \bar{u}_K \quad \mathbf{X} \in S_1, \quad (11)$$

$$n_K^0 x_{l,L} (T_{KL} - \rho_0 J^{-1} \Pi_K E_L) \delta_{lM} = \bar{p}_M \quad \mathbf{X} \in S_2, \quad (12)$$

where  $S_1 \cup S_2 = S$ ,  $S_1 \cap S_2 = 0$ , and  $S$  covers the total boundary;  $\bar{u}_K$  and  $\bar{p}_M$  are, respectively, the given displacement and traction on the boundary in the reference configuration;  $n_K^0(\mathbf{X})$  is the unit normal to the body in the reference configuration.

#### (b) Electrical boundary conditions

$$\phi = \bar{\phi} \quad \mathbf{X} \in S_3, \quad (13)$$

$$n_K^0 (J^{-1} \rho_0 \Pi_K + \varepsilon_0 E_K) = \bar{D}_{n^0} \quad \mathbf{X} \in S_4, \quad (14)$$

where  $S_3 \cup S_4 = S$ ,  $S_3 \cap S_4 = 0$ ;  $\bar{\phi}$  and  $\bar{D}_{n^0}$  are, respectively, the known electric potential and normal electric displacement on the boundary in the reference configuration.

#### (c) Initial conditions

$$u_K(\mathbf{X}, 0) = u_K^0(\mathbf{X}), \quad (15)$$

$$\dot{u}_K(\mathbf{X}, 0) = \dot{u}_K^0(\mathbf{X}), \quad (16)$$

where  $u_K^0$  is the known initial displacement and  $\dot{u}_K^0$  the known initial velocity.

## 3. Transversely isotropic materials with symmetry class 6mm

### 3.1. Polynomial integrity basis

Two basic requirements of invariance that must be imposed upon the constitutive equations are spatial invariance and material invariance (Jordan and Eringen 1964). For 6mm piezoelectricity with both the elastically symmetric axis and the poling direction as the  $X_3$ -axis, the polynomial integrity basis, the degree of which is less than three, can be given in the following concise form (Kiral and Eringen 1990).

Elements in  $\Gamma_{IJ}$  only:

$$\text{Degree 1: } \Gamma_{33}, \quad \Gamma_{11} + \Gamma_{22}, \quad (17)$$

$$\text{Degree 2: } \Gamma_{11}\Gamma_{22} - \Gamma_{12}^2, \quad \Gamma_{13}^2 + \Gamma_{23}^2, \quad (18)$$

$$\text{Degree 3: } \Gamma_{11}(\Gamma_{11}^2 + 6\Gamma_{11}\Gamma_{22} - 12\Gamma_{12}^2 + 9\Gamma_{22}^2), \quad \Gamma_{11}\Gamma_{23}^2 + \Gamma_{22}\Gamma_{13}^2 - \Gamma_{13}\Gamma_{23}\Gamma_{12}. \quad (19)$$

Elements in  $E_I$  only:

$$\text{Degree 1: } E_3, \quad (20)$$

$$\text{Degree 2: } E_1^2 + E_2^2. \quad (21)$$

Elements in  $\Gamma_{IJ}$  and  $E_I$  only:

$$\text{Degree 2: } \Gamma_{31}E_1 + \Gamma_{23}E_2, \quad (22)$$

$$\text{Degree 3: } (E_1\Gamma_{23} + E_2\Gamma_{31})\Gamma_{12} - E_1\Gamma_{22}\Gamma_{31} - E_2\Gamma_{11}\Gamma_{23}, \quad (23a)$$

$$\Gamma_{11}E_2^2 + \Gamma_{22}E_1^2 - 2E_1E_2\Gamma_{12}. \quad (23b)$$

### 3.2. Polynomial free energy function

In order to derive the second-order nonlinear constitutive equations, the energy density function  $\Sigma$  should be formed as a third-order polynomial function of  $\Gamma_{IJ}$  and  $E_I$ . Neglecting the initial stress and initial polarization, i.e. assuming that the energy density function of the piezoelectricity is zero when it is in a free state, from equations (17) to (23), after complicated symbolic mathematical manipulations using the Mathematica software package, the energy density function  $\Sigma$  can finally be obtained in the following form

$$\Sigma = \Sigma_a + \Sigma_\varepsilon + \Sigma_e + \Sigma_C + \Sigma_\eta + \Sigma_g + \Sigma_Q, \quad (24)$$

where

$$\Sigma_a = a_1 (\Gamma_{11}\Gamma_{22} - \Gamma_{12}^2) + a_2 (\Gamma_{23}^2 + \Gamma_{31}^2) + a_3 \Gamma_{33}^2 + a_4 (\Gamma_{11} + \Gamma_{22}) \Gamma_{33} + a_5 (\Gamma_{11} + \Gamma_{22})^2, \quad (25a)$$

$$\Sigma_\varepsilon = \varepsilon_1 (E_1^2 + E_2^2) + \varepsilon_2 E_3^2, \quad (25b)$$

$$\Sigma_e = e_1 (\Gamma_{31}E_1 + \Gamma_{23}E_2) + e_2 \Gamma_{33}E_3 + e_3 (\Gamma_{11} + \Gamma_{22}) E_3, \quad (25c)$$

$$\begin{aligned} \Sigma_C = & C_1 \Gamma_{11} (\Gamma_{11}^2 - 12\Gamma_{12}^2 + 6\Gamma_{11}\Gamma_{22} + 9\Gamma_{22}^2) \\ & + C_2 (\Gamma_{11}\Gamma_{23}^2 + \Gamma_{31} (\Gamma_{22}\Gamma_{31} - \Gamma_{12}\Gamma_{23})) \\ & + C_3 (\Gamma_{11}\Gamma_{22} - \Gamma_{12}^2) \Gamma_{33} + C_4 (\Gamma_{23}^2 + \Gamma_{31}^2) \Gamma_{33} \\ & + C_5 (\Gamma_{11} + \Gamma_{22}) (\Gamma_{11}\Gamma_{22} - \Gamma_{12}^2) \\ & + C_6 (\Gamma_{11} + \Gamma_{22}) (\Gamma_{23}^2 + \Gamma_{31}^2) + C_7 \Gamma_{33}^3 \\ & + C_8 (\Gamma_{11} + \Gamma_{22}) \Gamma_{33}^2 + C_9 (\Gamma_{11} + \Gamma_{22})^3 \\ & + C_{10} (\Gamma_{11} + \Gamma_{22})^2 \Gamma_{33}, \end{aligned} \quad (25d)$$

$$\Sigma_\eta = \eta_1 (E_1^2 + E_2^2) E_3 + \eta_2 E_3^3, \quad (25e)$$

$$\begin{aligned} \Sigma_g = & g_1 (\Gamma_{12}\Gamma_{23}E_1 - \Gamma_{22}\Gamma_{31}E_1 - \Gamma_{11}\Gamma_{23}E_2 + \Gamma_{12}\Gamma_{31}E_2) \\ & + g_2 \Gamma_{33} (\Gamma_{31}E_1 + \Gamma_{23}E_2) \\ & + g_3 (\Gamma_{11} + \Gamma_{22}) (\Gamma_{31}E_1 + \Gamma_{23}E_2) \\ & + g_4 (-\Gamma_{12}^2 + \Gamma_{11}\Gamma_{22}) E_3 + g_5 (\Gamma_{23}^2 + \Gamma_{31}^2) E_3 \\ & + g_6 \Gamma_{33}^2 E_3 + g_7 (\Gamma_{11} + \Gamma_{22})^2 E_3 \\ & + g_8 (\Gamma_{11} + \Gamma_{22}) \Gamma_{33} E_3, \end{aligned} \quad (25f)$$

$$\begin{aligned} \Sigma_Q = & Q_1 (\Gamma_{22}E_1^2 - 2\Gamma_{12}E_1E_2 + \Gamma_{11}E_2^2) \\ & + Q_2 \Gamma_{33} (E_1^2 + E_2^2) + Q_3 (\Gamma_{11} + \Gamma_{22}) \\ & \times (E_1^2 + E_2^2) + Q_4 (\Gamma_{31}E_1 + \Gamma_{23}E_2) E_3 \\ & + Q_5 \Gamma_{33} E_3^2 + Q_6 (\Gamma_{11} + \Gamma_{22}) E_3^2. \end{aligned} \quad (25g)$$

Equation (24) indicates that the energy density consists of seven parts. Obviously,  $\Sigma_a$ ,  $\Sigma_\varepsilon$ , and  $\Sigma_e$  correspond to the linear constitutive relations, and  $\Sigma_C$ ,  $\Sigma_\eta$ ,  $\Sigma_g$ , and  $\Sigma_Q$  correspond to the nonlinear constitutive relations. Also, it is easily observed that there are a total of 36 independent material constants for the  $6mm$  crystal class, which is in agreement with the early literature (Landolt 1966), and that there are ten independent constants for the corresponding linear material, which is further in agreement with the well-known results.

### 3.3. Second-order constitutive theory

Substituting equation (24) together with equation (25) into equations (9) and (10), we obtain the elastic stress and electric

polarization as follows

$$T_{IJ} = T_{IJa} + T_{IJe} + T_{IJc} + T_{IJg} + T_{IJQ}, \quad (26)$$

$$\Pi_I = \Pi_{I\varepsilon} + \Pi_{Ie} + \Pi_{I\eta} + \Pi_{Ig} + \Pi_{IQ}, \quad (27)$$

where

$$T_{11a} = a_1 \Gamma_{22} + a_4 \Gamma_{33} + 2a_5 (\Gamma_{11} + \Gamma_{22}), \quad (28a)$$

$$T_{11e} = e_3 E_3, \quad (28b)$$

$$\begin{aligned} T_{11c} = & 3C_1 (\Gamma_{11}^2 - 4\Gamma_{12}^2 + 4\Gamma_{11}\Gamma_{22} + 3\Gamma_{22}^2) \\ & + C_2 \Gamma_{23}^2 + C_3 \Gamma_{22}\Gamma_{33} + C_5 (2\Gamma_{11}\Gamma_{22} + \Gamma_{22}^2 - \Gamma_{12}^2) \\ & + C_6 (\Gamma_{23}^2 + \Gamma_{31}^2) + C_8 \Gamma_{33}^2 - 3C_9 (\Gamma_{11} + \Gamma_{22})^2 \\ & + 2C_{10} (\Gamma_{11} + \Gamma_{22}) \Gamma_{33}, \end{aligned} \quad (28c)$$

$$\begin{aligned} T_{11g} = & -g_1 \Gamma_{23}E_2 + g_3 (\Gamma_{31}E_1 + \Gamma_{23}E_2) \\ & + g_4 \Gamma_{22}E_3 + 2g_7 (\Gamma_{11} + \Gamma_{22}) E_3 + g_8 \Gamma_{33}E_3, \end{aligned} \quad (28d)$$

$$T_{11Q} = Q_1 E_2^2 + Q_3 (E_1^2 + E_2^2) + Q_6 E_3^2, \quad (28e)$$

$$T_{22a} = a_1 \Gamma_{11} + a_4 \Gamma_{33} + 2a_5 (\Gamma_{11} + \Gamma_{22}), \quad (29a)$$

$$T_{22e} = e_3 E_3, \quad (29b)$$

$$\begin{aligned} T_{22c} = & 6C_1 \Gamma_{11} (\Gamma_{11} + 3\Gamma_{22}) + C_2 \Gamma_{31}^2 \\ & + C_3 \Gamma_{11}\Gamma_{33} + C_5 (2\Gamma_{11}\Gamma_{22} + \Gamma_{11}^2 - \Gamma_{12}^2) \\ & + C_6 (\Gamma_{23}^2 + \Gamma_{31}^2) + C_8 \Gamma_{33}^2 + 3C_9 (\Gamma_{11} + \Gamma_{22})^2 \\ & + 2C_{10} (\Gamma_{11} + \Gamma_{22}) \Gamma_{33}, \end{aligned} \quad (29c)$$

$$\begin{aligned} T_{22g} = & -g_1 \Gamma_{31}E_1 + g_3 (\Gamma_{31}E_1 + \Gamma_{23}E_2) \\ & + g_4 \Gamma_{11}E_3 + 2g_7 (\Gamma_{11} + \Gamma_{22}) E_3 + g_8 \Gamma_{33}E_3, \end{aligned} \quad (29d)$$

$$T_{22Q} = Q_1 E_1^2 + Q_3 (E_1^2 + E_2^2) + Q_6 E_3^2, \quad (29e)$$

$$T_{33a} = 2a_3 \Gamma_{33} + a_4 (\Gamma_{11} + \Gamma_{22}), \quad (30a)$$

$$T_{33e} = e_2 E_3, \quad (30b)$$

$$\begin{aligned} T_{33c} = & C_3 (\Gamma_{11}\Gamma_{22} - \Gamma_{12}^2) + C_4 (\Gamma_{23}^2 + \Gamma_{31}^2) \\ & + 3C_7 \Gamma_{33}^2 + 2C_8 (\Gamma_{11} + \Gamma_{22}) \Gamma_{33} \\ & + C_{10} (\Gamma_{11} + \Gamma_{22})^2, \end{aligned} \quad (30c)$$

$$\begin{aligned} T_{33g} = & g_2 (\Gamma_{31}E_1 + \Gamma_{23}E_2) + 2g_6 \Gamma_{33}E_3 \\ & + g_8 (\Gamma_{11} + \Gamma_{22}) E_3, \end{aligned} \quad (30d)$$

$$T_{33Q} = Q_2 (E_1^2 + E_2^2) + Q_5 E_3^2, \quad (30e)$$

$$T_{23a} = a_2 \Gamma_{23}, \quad (31a)$$

$$T_{23e} = 0.5e_1 E_2, \quad (31b)$$

$$\begin{aligned} T_{23c} = & C_2 (\Gamma_{11}\Gamma_{23} - 0.5\Gamma_{12}\Gamma_{31}) \\ & + C_4 \Gamma_{23}\Gamma_{33} + C_6 (\Gamma_{11} + \Gamma_{22}) \Gamma_{23}, \end{aligned} \quad (31c)$$

$$\begin{aligned} T_{23g} = & 0.5g_1 (\Gamma_{12}E_1 - \Gamma_{11}E_2) + 0.5g_2 \Gamma_{33}E_2 \\ & + 0.5g_3 (\Gamma_{11} + \Gamma_{22}) E_2 + g_5 \Gamma_{23}E_3, \end{aligned} \quad (31d)$$

$$T_{23d} = 0.5Q_4 E_2 E_3, \quad (31e)$$

$$T_{31a} = a_2 \Gamma_{31}, \quad (32a)$$

$$T_{31e} = 0.5e_1 E_1, \quad (32b)$$

$$\begin{aligned} T_{31c} = & C_2 (\Gamma_{22}\Gamma_{31} - 0.5\Gamma_{12}\Gamma_{23}) + C_4 \Gamma_{31}\Gamma_{33} \\ & + C_6 (\Gamma_{11} + \Gamma_{22}) \Gamma_{31}, \end{aligned} \quad (32c)$$

$$\begin{aligned} T_{31g} = & 0.5g_1 (\Gamma_{12}E_2 - \Gamma_{22}E_1) + 0.5g_2 \Gamma_{33}E_1 \\ & + 0.5g_3 (\Gamma_{11} + \Gamma_{22}) E_1 + g_5 \Gamma_{31}E_3, \end{aligned} \quad (32d)$$

$$T_{31Q} = 0.5Q_4 E_1 E_3, \quad (32e)$$

$$T_{12a} = -a_1 \Gamma_{12}, \quad (33a)$$

$$T_{12c} = -12C_1 \Gamma_{11} \Gamma_{12} - 0.5C_2 \Gamma_{23} \Gamma_{31} - C_3 \Gamma_{12} \Gamma_{33} - C_4 \Gamma_{12} (\Gamma_{11} + \Gamma_{12}), \quad (33b)$$

$$T_{12e} = 0, \quad (33c)$$

$$T_{12g} = 0.5g_1 (\Gamma_{23} E_1 + \Gamma_{31} E_2), \quad (33d)$$

$$T_{12Q} = -Q_1 E_1 E_2, \quad (33e)$$

$$\Pi_{1\varepsilon} = -2\varepsilon_1 E_1, \quad (34a)$$

$$\Pi_{1e} = -e_1 \Gamma_{31}, \quad (34b)$$

$$\Pi_{1\eta} = -2\eta_1 E_1 E_3, \quad (34c)$$

$$\Pi_{1g} = -g_1 (\Gamma_{12} \Gamma_{23} - \Gamma_{22} \Gamma_{31}) - g_2 \Gamma_{31} \Gamma_{33} - g_3 (\Gamma_{11} + \Gamma_{22}) \Gamma_{31}, \quad (34d)$$

$$\Pi_{1Q} = 2Q_1 (\Gamma_{22} E_1 - \Gamma_{12} E_2) - 2Q_2 \Gamma_{33} E_1 - 2Q_3 (\Gamma_{11} + \Gamma_{22}) E_1 - Q_4 \Gamma_{31} E_3, \quad (34e)$$

$$\Pi_{2\varepsilon} = -2\varepsilon_1 E_2, \quad (35a)$$

$$\Pi_{2e} = -e_1 \Gamma_{23}, \quad (35b)$$

$$\Pi_{2\eta} = -2\eta_1 E_2 E_3, \quad (35c)$$

$$\Pi_{2g} = -g_1 (\Gamma_{12} \Gamma_{31} - \Gamma_{11} \Gamma_{23}) - g_2 \Gamma_{23} \Gamma_{33} - g_3 (\Gamma_{11} + \Gamma_{22}) \Gamma_{23}, \quad (35d)$$

$$\Pi_{2Q} = 2Q_1 (\Gamma_{11} E_2 - \Gamma_{12} E_1) - 2Q_2 \Gamma_{33} E_2 - 2Q_3 (\Gamma_{11} + \Gamma_{22}) E_2 - Q_4 \Gamma_{23} E_3, \quad (35e)$$

$$\Pi_{3\varepsilon} = -2\varepsilon_2 E_3, \quad (36a)$$

$$\Pi_{3e} = -e_2 \Gamma_{33} - e_3 (\Gamma_{11} + \Gamma_{22}), \quad (36b)$$

$$\Pi_{3\eta} = -\eta_1 (E_1^2 + E_2^2) - 3\eta_2 E_3^2, \quad (36c)$$

$$\Pi_{3g} = -g_4 (\Gamma_{11} \Gamma_{22} - \Gamma_{12}^2) - g_5 (\Gamma_{23}^2 + \Gamma_{31}^2) - g_6 \Gamma_{33}^2 - g_7 (\Gamma_{11} + \Gamma_{22})^2 - g_8 (\Gamma_{11} + \Gamma_{22}) \Gamma_{33}, \quad (36d)$$

$$\Pi_{3Q} = -Q_4 (\Gamma_{31} E_1 + \Gamma_{23} E_2) - 2Q_5 \Gamma_{33} E_3 - 2Q_6 (\Gamma_{11} + \Gamma_{22}) E_3. \quad (36e)$$

Equations (28)–(36) can easily be written in matrix forms. Thus, we have obtained the concise expressions of nonlinear constitutive equations for the  $6mm$  crystal class, which is the basis for analyzing the nonlinear problems of piezoelectric materials with this kind of symmetry.

It should also be pointed out that the corresponding results of small deformations and weak electric fields (Yang and Batra 1995) and the corresponding results of small deformations and strong fields (Tiersten 1993, Yang and Batra 1995) can easily be deduced from equations (26)–(36).

#### 4. Cubic materials with symmetry class $m3$

For  $m3$  piezoelectricity, the polynomial integrity basis, the degree of which is less than three, is given by (Kiral and Eringen 1990).

Elements in  $\Gamma_{IJ}$  only:

$$\text{Degree 1: } \Gamma_{11} + \Gamma_{22} + \Gamma_{33}, \quad (37)$$

$$\text{Degree 2: } \Gamma_{11} \Gamma_{22} + \Gamma_{22} \Gamma_{33} + \Gamma_{33} \Gamma_{11}, \quad (38)$$

$$\Gamma_{23}^2 + \Gamma_{31}^2 + \Gamma_{12}^2,$$

$$\text{Degree 3: } \Gamma_{11} \Gamma_{22} \Gamma_{33}, \quad \Gamma_{23} \Gamma_{31} \Gamma_{12}, \quad (39a)$$

$$\Gamma_{11} \Gamma_{23}^2 + \Gamma_{22} \Gamma_{31}^2 + \Gamma_{33} \Gamma_{12}^2, \quad (39b)$$

$$\Gamma_{11} (\Gamma_{31}^2 - \Gamma_{12}^2) + \Gamma_{22} (\Gamma_{12}^2 - \Gamma_{23}^2) + \Gamma_{33} (\Gamma_{23}^2 - \Gamma_{31}^2), \quad (39c)$$

$$\Gamma_{11} \Gamma_{22} (\Gamma_{11} - \Gamma_{22}) + \Gamma_{22} \Gamma_{33} (\Gamma_{22} - \Gamma_{33}) + \Gamma_{33} \Gamma_{11} (\Gamma_{33} - \Gamma_{11}).$$

Elements in  $E_I$  only:

$$\text{Degree 2: } E_1^2 + E_2^2 + E_3^2. \quad (40)$$

Elements in  $\Gamma_{IJ}$  and  $E_I$  only:

$$\text{Degree 3: } E_2 E_3 \Gamma_{23} + E_3 E_1 \Gamma_{31} + E_1 E_2 \Gamma_{12}, \quad (41a)$$

$$E_1^2 \Gamma_{11} + E_2^2 \Gamma_{22} + E_3^2 \Gamma_{33}, \quad (41b)$$

$$E_1^2 (\Gamma_{22} - \Gamma_{33}) + E_2^2 (\Gamma_{33} - \Gamma_{11}) + E_3^2 (\Gamma_{11} - \Gamma_{22}).$$

Similarly, the polynomial energy density function can be expressed as

$$\Sigma = \Sigma_a + \Sigma_\varepsilon + \Sigma_C + \Sigma_Q, \quad (42)$$

where

$$\Sigma_a = a_1 (\Gamma_{11} + \Gamma_{22} + \Gamma_{33})^2 + a_2 (\Gamma_{22} \Gamma_{33} + \Gamma_{33} \Gamma_{11} + \Gamma_{11} \Gamma_{22}) + a_3 (\Gamma_{23}^2 + \Gamma_{31}^2 + \Gamma_{12}^2), \quad (43a)$$

$$\Sigma_C = C_1 (\Gamma_{11} + \Gamma_{22} + \Gamma_{33})^3 + C_2 (\Gamma_{11} + \Gamma_{22} + \Gamma_{33}) \times (\Gamma_{22} \Gamma_{33} + \Gamma_{33} \Gamma_{11} + \Gamma_{11} \Gamma_{22}) + C_3 (\Gamma_{11} + \Gamma_{22} + \Gamma_{33}) (\Gamma_{23}^2 + \Gamma_{31}^2 + \Gamma_{12}^2) + C_4 \Gamma_{11} \Gamma_{22} \Gamma_{33} + C_5 \Gamma_{12} \Gamma_{23} \Gamma_{31} + C_6 (\Gamma_{11} \Gamma_{23}^2 + \Gamma_{22} \Gamma_{31}^2 + \Gamma_{33} \Gamma_{12}^2) + C_7 (\Gamma_{12}^2 \Gamma_{22} - \Gamma_{23}^2 \Gamma_{22} + \Gamma_{31}^2 \Gamma_{11} - \Gamma_{12}^2 \Gamma_{11} + \Gamma_{23}^2 \Gamma_{33} - \Gamma_{31}^2 \Gamma_{33}) + C_8 (\Gamma_{11} - \Gamma_{22}) (\Gamma_{11} - \Gamma_{33}) (\Gamma_{22} - \Gamma_{33}), \quad (43b)$$

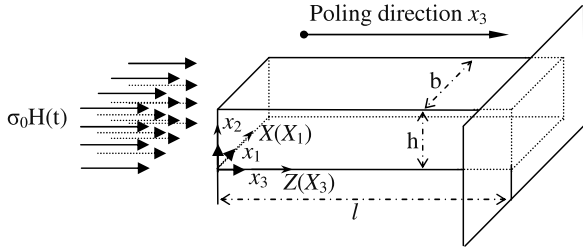
$$\Sigma_\varepsilon = \varepsilon_1 (E_1^2 + E_2^2 + E_3^2), \quad (43c)$$

$$\Sigma_Q = Q_1 (\Gamma_{11} + \Gamma_{22} + \Gamma_{33}) (E_1^2 + E_2^2 + E_3^2) + Q_2 (\Gamma_{12} E_1 E_2 + \Gamma_{31} E_1 E_3 + \Gamma_{23} E_2 E_3) + Q_3 ((\Gamma_{22} - \Gamma_{33}) E_1^2 + (\Gamma_{33} - \Gamma_{11}) E_2^2 + (\Gamma_{11} - \Gamma_{22}) E_3^2) + Q_4 (\Gamma_{11} E_1^2 + \Gamma_{22} E_2^2 + \Gamma_{33} E_3^2). \quad (43d)$$

Substituting equations (42) and (43) into equations (9) and (10), we finally obtain the elastic stress and electric polarization as follows

$$T_{IJ} = T_{IJa} + T_{IJC} + T_{IJQ}, \quad (44)$$

$$\Pi_I = \Pi_{I\varepsilon} + \Pi_{IQ}, \quad (45)$$



**Figure 1.** A one-dimensional piezoelectric model of 6mm crystal class loaded at the left end along the poling direction.

where

$$T_{11a} = 2a_1 (\Gamma_{11} + \Gamma_{22} + \Gamma_{33}) + a_2 (\Gamma_{22} + \Gamma_{33}), \quad (46a)$$

$$\begin{aligned} T_{11c} = & 3C_1 (\Gamma_{11} + \Gamma_{22} + \Gamma_{33})^2 \\ & + C_2 ((\Gamma_{22} + \Gamma_{33}) (\Gamma_{11} + \Gamma_{22} + \Gamma_{33}) + \Gamma_{11}\Gamma_{22} \\ & + \Gamma_{11}\Gamma_{33} + \Gamma_{22}\Gamma_{33}) + C_3 (\Gamma_{12}^2 + \Gamma_{23}^2 + \Gamma_{31}^2) \\ & + C_4 \Gamma_{22}\Gamma_{33} + C_6 \Gamma_{23}^2 + C_7 (\Gamma_{31}^2 - \Gamma_{12}^2) \\ & + C_8 (2\Gamma_{11}\Gamma_{22} - 2\Gamma_{11}\Gamma_{33} + \Gamma_{33}^2 - \Gamma_{22}^2), \end{aligned} \quad (46b)$$

$$T_{11Q} = Q_1 (E_1^2 + E_2^2 + E_3^2) + Q_3 (E_3^2 - E_2^2) + Q_4 E_1^2, \quad (46c)$$

$$T_{23a} = a_3 \Gamma_{23}, \quad (47a)$$

$$\begin{aligned} T_{23c} = & C_3 \Gamma_{23} (\Gamma_{11} + \Gamma_{22} + \Gamma_{33}) + 0.5C_5 \Gamma_{31} \Gamma_{12} \\ & + C_6 \Gamma_{11} \Gamma_{23} + C_7 \Gamma_{23} (\Gamma_{33} - \Gamma_{22}), \end{aligned} \quad (47b)$$

$$T_{23Q} = 0.5Q_2 E_2 E_3, \quad (47c)$$

$$\Pi_{1\varepsilon} = -2\varepsilon_1 E_1, \quad (48a)$$

$$\begin{aligned} \Pi_{1Q} = & -2Q_1 (\Gamma_{11} + \Gamma_{22} + \Gamma_{33}) E_1 - Q_2 (\Gamma_{12} E_2 + \Gamma_{31} E_3) \\ & - 2Q_3 (\Gamma_{22} - \Gamma_{33}) E_1 - 2Q_4 \Gamma_{11} E_1. \end{aligned} \quad (48b)$$

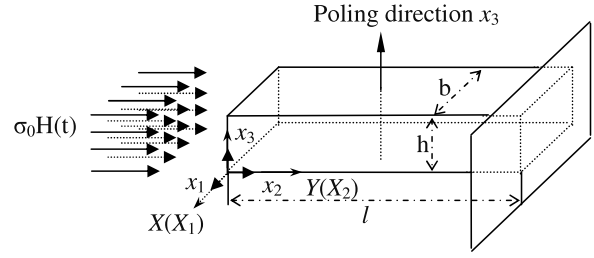
The other stress and polarization components can be obtained by simple index permutations, which are omitted here for brevity.

As shown in equations (46)–(48), for linear cubic piezoelectricity, there are five independent material constants, which is in agreement with the well-known results. It is interesting to note that for the nonlinear  $m3$  crystal class, the squared terms of strain and/or electric field components have no effects on the electric polarization, whilst the products of strain and electric field components have no contribution to the stress distribution. In addition, the analysis on the cubic system with  $m3$  crystal class also shows that even for nonlinear materials, there are only a total of 16 independent material constants.

Furthermore, we remark that if  $C_7$ ,  $C_8$ , and  $Q_3$  are all set to be zero, then equations (46)–(48) directly reduce to the corresponding constitutive equations of the cubic system with the symmetry class  $m3m$ .

## 5. One-dimensional models of nonlinear impacts for the 6mm crystal class

As shown in figures 1 and 2, a bar of rectangular cross-section with length  $l$  is fixed at the right end. In this section, we will derive the simplified equations of one-dimensional impact problems under two kinds of mechanical impact loadings.



**Figure 2.** A one-dimensional piezoelectric model of 6mm crystal class loaded at the left end normal to the poling direction.

### 5.1. Mechanical loads parallel to the poling direction

In this case, as shown in figure 1,  $x_3 = X_3 + w(X_3, t) = Z + w(Z, t)$ ,  $u_3 = w(Z, t)$ ,  $\phi = \phi(Z, t)$ , the constitutive equations can be directly simplified from the three-dimensional ones as

$$T_{33} = a_{33} \Gamma_{33} - e_{33} E_3 + \frac{1}{2} C_{333} \Gamma_{33}^2 - \frac{1}{2} Q_{333} E_3^2 - g_{333} \Gamma_{33} E_3, \quad (49)$$

$$\Pi_3 = e_{33} \Gamma_{33} + \varepsilon_{33} E_3 + \frac{1}{2} g_{333} \Gamma_{33}^2 + \frac{1}{2} \eta_{333} E_3^2 + Q_{333} \Gamma_{33} E_3, \quad (50)$$

where  $a_{33}$ ,  $e_{33}$ ,  $\varepsilon_{33}$ ,  $C_{333}$ ,  $g_{333}$ ,  $Q_{333}$ , and  $\eta_{333}$  are the new and independent material constants, which are introduced for clarity. Also,

$$\Gamma_{33}(Z, t) = \frac{\partial w}{\partial Z} + \frac{1}{2} \left( \frac{\partial w}{\partial Z} \right)^2, \quad (51)$$

$$E_3(Z, t) = -\frac{\partial \phi}{\partial Z}. \quad (52)$$

The governing equations can finally be expressed as

$$\begin{aligned} T_{33,Z} \left( 1 + \frac{dw}{\partial Z} \right) + T_{33} \frac{d^2 w}{\partial Z^2} + \varepsilon_0 E_3 E_{3,Z} \left( 1 + \frac{dw}{\partial Z} \right)^{-2} \\ - \varepsilon_0 E_3^2 \frac{d^2 w}{\partial Z^2} \left( 1 + \frac{dw}{\partial Z} \right)^{-3} = \rho_0 \ddot{w}, \end{aligned} \quad (53)$$

$$\begin{aligned} \Pi_{3,Z} - \varepsilon_0 \left( 1 + \frac{dw}{\partial Z} \right)^{-2} \frac{d^2 w}{\partial Z^2} E_3 \\ + \varepsilon_0 \left( 1 + \frac{dw}{\partial Z} \right)^{-1} E_{3,Z} = 0. \end{aligned} \quad (54)$$

For the mechanical impact only, the mechanical and electric boundary conditions are given as

$$\begin{aligned} T_{33}(0, t) \left( 1 + \frac{dw(0, t)}{dZ} \right) - \rho_0(0) \Pi_3(0, t) E_3(0, t) \\ = -\sigma_0 H(t), \end{aligned} \quad (55a)$$

$$w(l, t) = 0, \quad (55b)$$

$$\left( 1 + \frac{dw(0, t)}{dZ} \right) \rho_0(0) \Pi_3(0, t) + \varepsilon_0 E_3(0, t) = 0, \quad (56a)$$

$$\left( 1 + \frac{dw(l, t)}{dZ} \right) \rho_0(l) \Pi_3(l, t) + \varepsilon_0 E_3(l, t) = 0, \quad (56b)$$

where  $\sigma_0$  is the known constant and  $H(t)$  the Heaviside unit step function.



**Table 1.** Nonlinear piezoelectric coefficients for quartz.

Name	Present	D&G <sup>a</sup>	Value
Second-order elastic stiffness (GPa)	$a_{33}$	$C_{33}^E$	$8.6736 \times 10^{10b}$
Piezoelectric coupling (C m <sup>-2</sup> )	$e_{33}$	$e_{33}^\eta$	$0.171^c$
Dielectric constant ( $\epsilon^{0d}$ )	$\epsilon_{33}$	$\epsilon_{33}^\eta$	$4.40^e$
Third-order elastic (GPa)	$C_{333}$	$C_{333}^E$	$-30.0 \times 10^{10f}$
Third-order piezoelectric ( $\epsilon^0$ m V <sup>-1</sup> )	$g_{333}$	$1/2e_{ijkml}$	$-1.31^g$
Electrostrictive ( $\epsilon^0$ F m <sup>-1</sup> )	$Q_{333}$	$f_{333}$	$-4.40^h$
Third-order dielectric (F V <sup>-1</sup> )	$\eta_{333}$	$\epsilon_{333}^\eta$	$O(-3.5 \times 10^{-17})^i$

<sup>a</sup> D & G\*: Davison and Graham (1979). <sup>b</sup> Value for quartz from COMSOL 3.5a Material Library. <sup>c</sup> Value from D&G.

<sup>d</sup>  $\epsilon^0 = 8.854 \times 10^{-12}$  F m<sup>-1</sup> (electric constant in vacuum).

<sup>e</sup> Relative dielectric constant value, references to Bechmann (1958) and Fontanella and Andeen (1974).

<sup>f</sup> Same order as the (second-order) elastic stiffness but significantly large for finite strain, reference to D&G.

<sup>g</sup> The contribution is typically several orders smaller than other terms, reference to D&G.

<sup>h</sup> The electrostrictive coefficient is typically the same order as the second-order dielectric but of opposite sign.

<sup>i</sup> Several orders smaller than other coefficients and can be neglected unless the  $E$ -field is extremely high, e.g. several orders larger than the strain.

The initial conditions can be expressed in terms of the known displacement  $w^0(Z)$  and velocity  $\dot{w}^0(Z)$  as follows

$$w(Z, 0) = w^0(Z), \quad (57a)$$

$$\dot{w}(Z, 0) = \dot{w}^0(Z). \quad (57b)$$

It should be noted that, as shown in equations (49) and (50), when the loading direction is in the poling direction, there are a total of seven independent material constants, which include three linear coefficients (i.e.  $a_{33}$ ,  $e_{33}$ , and  $\epsilon_{33}$ ) and four nonlinear coefficients (i.e.  $C_{333}$ ,  $g_{333}$ ,  $Q_{333}$ , and  $\eta_{333}$ ).

### 5.2. Mechanical loads vertical to the poling direction

In this case, as shown in figure 2,  $x_2 = Y + v(Y, t)$ ,  $u_2 = v(Y, t)$ ,  $\phi = \phi(Y, t)$ , the constitutive equations are obtained as

$$T_{22} = a_{11}\Gamma_{22} + \frac{1}{2}C_{222}\Gamma_{22}^2 - \frac{1}{2}Q_{222}E_2^2, \quad (58)$$

$$\Pi_2 = \epsilon_{11}E_2 + Q_{222}\Gamma_{22}E_2, \quad (59)$$

where  $a_{11}$ ,  $\epsilon_{11}$ ,  $C_{222}$ , and  $Q_{222}$  are the new material constants introduced here for clarity. Also,

$$\Gamma_{22}(Y, t) = \frac{\partial v}{\partial Y} + \frac{1}{2} \left( \frac{\partial v}{\partial Y} \right)^2, \quad (60)$$

$$E_2(Y, t) = -\frac{\partial \phi}{\partial Y}. \quad (61)$$

The governing equations can finally be expressed as

$$T_{22,Y} \left( 1 + \frac{dv}{dY} \right) + T_{22} \frac{d^2v}{dY^2} + \epsilon_0 E_2 E_{2,Y} \left( 1 + \frac{dv}{dY} \right)^{-2} - \epsilon_0 E_2^2 \frac{d^2v}{dY^2} \left( 1 + \frac{dv}{dY} \right)^{-3} = \rho_0 \ddot{v}, \quad (62)$$

$$\begin{aligned} \Pi_{2,Y} - \epsilon_0 \left( 1 + \frac{dv}{dY} \right)^{-2} \frac{d^2v}{dY^2} E_2 \\ + \epsilon_0 \left( 1 + \frac{dv}{dY} \right)^{-1} E_{2,Y} = 0. \end{aligned} \quad (63)$$

Correspondingly, the conditions of unique solution can be described as

$$T_{22}(0, t) \left( 1 + \frac{dv(0, t)}{dY} \right) - \rho_0(0) \Pi_2(0, t) E_2(0, t) = -\sigma_0 H(t), \quad (64a)$$

$$v(l, t) = 0, \quad (64b)$$

$$\left( 1 + \frac{dv(0, t)}{dY} \right) \rho_0(0) \Pi_2(0, t) + \epsilon_0 E_2(0, t) = 0, \quad (65a)$$

$$\left( 1 + \frac{dv(l, t)}{dY} \right) \rho_0(l) \Pi_2(l, t) + \epsilon_0 E_2(l, t) = 0, \quad (65b)$$

$$v(Y, 0) = v^0(Y), \quad (66a)$$

$$\dot{v}(Y, 0) = \dot{v}^0(Y), \quad (66b)$$

where  $v^0(Y)$  and  $\dot{v}^0(Y)$  are, respectively, the known initial displacement and velocity.

As shown in equations (58) and (59), when the loading direction is vertical to the poling direction, there are a total of four independent material constants, which include two linear coefficients (i.e.  $a_{11}$  and  $\epsilon_{11}$ ) and two nonlinear coefficients (i.e.  $C_{222}$  and  $Q_{222}$ ).

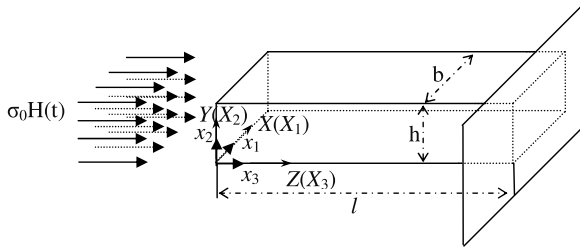
## 6. One-dimensional model of nonlinear impacts for the $m3$ crystal class

For the one-dimensional  $m3$  crystal class structure, if the applied mechanical loads are parallel to the  $X_3(Z)$  axis (see figure 3), we have  $x_3 = X_3 + w(X_3, t) = Z + w(Z, t)$ ,  $u_3 = w(Z, t)$ ,  $\phi = \phi(Z, t)$ .

Similar to the  $6mm$  crystal class, the governing equations (53) and (54), the extended geometry equations (51) and (52), and the conditions of unique solution (55)–(57) all remain the same. The constitutive equations can be expressed as

$$T_{33} = a_{33}\Gamma_{33} + \frac{1}{2}C_{333}\Gamma_{33}^2 - \frac{1}{2}Q_{333}E_3^2, \quad (67)$$





**Figure 3.** A one-dimensional piezoelectric model of  $m3$  crystal class loaded at the left end.

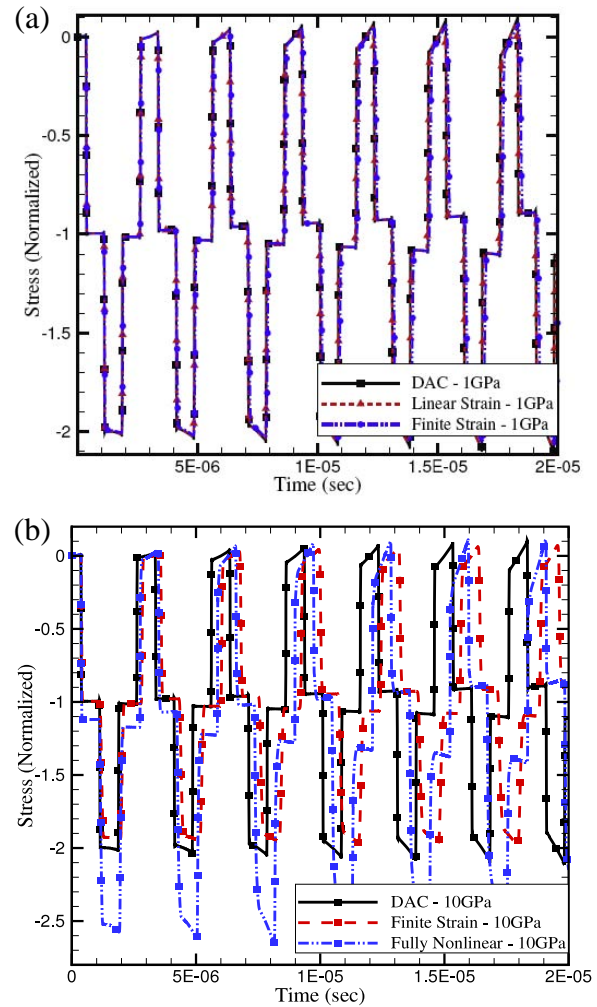
$$\Pi_3 = \varepsilon_{33} E_3 + Q_{333} \Gamma_{33} E_3. \quad (68)$$

As shown in equations (58) and (59), for the one-dimensional  $m3$  crystal class structure, there are a total of four independent material constants, which include two linear coefficients ( $a_{33}$  and  $\varepsilon_{33}$ ) and two nonlinear coefficients ( $C_{333}$  and  $Q_{333}$ ).

## 7. Numerical results

From the governing equations, equations (1) and (2), it is seen that for a one-dimensional response, the only change between crystal classes is the non-zero constants in the constitutive law which are different for different crystal classes. This has been explicitly shown for the  $6mm$  and  $3m$  crystal classes in section 6. We point out that experimental values for the nonlinear coefficients are, in general, not readily available for most materials. However, values for quartz, which is in the 32 crystal class, are available (Davison and Graham 1979). Consequently, for the illustrative purpose, equations (53) and (54) were solved numerically using quartz properties. Although, in general, the coefficients in equations (28)–(36), even for small deformations, are not the same as the classical constitutive coefficients (Feng *et al* 2009), in the one-dimensional case, however, there is a direct correspondence. This correspondence between those adopted in this paper and those in Davison and Graham (1979) is shown in table 1. These values were used when solving equations (53) and (54) using the COMSOL solver (COMSOL 2008) via the nonlinear constitutive relations (49) and (50). To reduce numerical noise, Rayleigh damping was added via an additional weak form term. In the numerical solutions, three different models are considered: (1) the Dubner–Abate–Crump (DAC) model for the linear small strain solved via Laplace transform techniques using a modified DAC algorithm (Lavery and Gazonas 2005); (2) the finite strain model where the finite strain terms in the governing equations and constitutive relations equation (49)–(51) are included in the solution but nonlinear effects due to the electric field are ignored; (3) the full nonlinear model where the fully nonlinear governing equations (53) and (54), along with the nonlinear constitutive relations (equations (49) and (50)), are solved using the corresponding material properties in table 1. As mentioned, the solutions for the second and third models were obtained by implementing the relevant equations in COMSOL (COMSOL 2008).

First, a step pressure load of  $\sigma_0 = 1$  GPa is applied at the left end of the piezoelectric quartz bar and the stress wave



**Figure 4.** One-dimensional stress wave response in the midpoint to a step pressure loading in the nonlinear piezoelectric quartz bar: a load of  $\sigma_0 = 1$  Pa based on the DAC, linear strain, and finite strain models in (a), and a load of  $\sigma_0 = 10$  GPa based on the DAC, finite strain, and full nonlinear models in (b).

(This figure is in colour only in the electronic version)

response at the middle point ( $l/2$ ) is calculated (figure 1) at different times. The results for the three models are shown in figure 4(a). It is observed that, for the infinitesimal strain deformation, the numerical result via COMSOL is identical to the analytical solution using the modified DAC. This indicates that the addition of the Rayleigh damping does not adversely affect the solution. It is also noted that the solution based on the finite strain model via the COMSOL solver is also very close to the linear strain modified DAC solution although there is a slight phase shift in the response. This clearly illustrates that quartz continues to respond linearly up to moderately large pressures.

Second, the pressure load is increased to  $\sigma_0 = 10$  GPa, which corresponds to a pressure value that is typical of shock loading, and the stress wave responses in the middle point of the bar are calculated (figure 4(b)) for the three models. It is seen that at this loading level the response exhibits a significant phase shift, due to the coupling and nonlinearity in

the constitutive relations (Lysne 1972). It is further observed that at a high loading, the amplitude of the stress wave can also be significantly increased due to the piezoelectric nonlinearity. It is further interesting to observe from figure 4(b) that the finite strain model has a wave speed slower than that in the full nonlinear model, and that waves in both nonlinear models are slower than that in the corresponding linear strain model. Whether this predicted effect on the wave speed occurs at finite strains remains to be experimentally validated.

## 8. Conclusions

In this paper, we have derived the three-dimensional constitutive equations for second-order nonlinear piezoelectricity with 6mm crystal class and m3 crystal class. As an application, the mathematical models of one-dimensional impact problems are also completely described. The one-dimensional nonlinear equations were then solved numerically via COMSOL and a significant effect of the piezoelectric nonlinearity on the phase and amplitude of the stress wave was clearly observed. Therefore, this work forms the basis for the development of nonlinear finite element codes for the analysis of dynamically loaded structures composed of piezoelectric ceramic with the symmetry class 6mm and/or symmetry class m3.

## Acknowledgments

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